

# Completion of Newton's Iterations Initialized at a Quasi-Universal Set

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## Abstract

Recently Schleicher and Stoll proposed efficient initialization of Newton's iterations. Given a black box subroutine for the evaluation of the Newton's ratio of a polynomial and its derivative, their algorithm very fast approximates all roots of a univariate polynomial except for a small fraction of them. Our recipes for the approximation of the remaining roots within the same asymptotic computational cost should answer the authors' challenge. Our work can be of independent interest as an example of synergistic variation and combination of polynomial root-finding methods towards enhancing their power.

**Key Words:** Polynomial roots; Newton iteration; Universal initial set; Quasi-universal set; Deflation; Maps of the variable; Functional iterations

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## 1 Introduction: the Problem

The paper [HSS01] proposed an ingenious initialization of Newton's iterations

$$y_0 = c, \quad y^{(h+1)} = y^{(h)} - p(y^{(h)})/p'(y^{(h)}), \quad h = 0, 1, \dots, \quad (1)$$

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for the approximation of all  $d$  roots of a univariate polynomial

$$p(x) = \sum_{i=0}^d p_i x^i = p_d \prod_{j=1}^d (x - x_j), \quad p_d \neq 0, \quad |x_j| \leq 1, \quad \text{for all } j, \quad (2)$$

given by a subroutine for the evaluation of the Newton's ratio

$$N_p(x) = p(x)/p'(x) \quad (3)$$

at a complex point  $x$ ; one can ensure that all roots  $x_j$  lie in the unit disc  $D(0, 1) = \{x : |x| \leq 1\}$  by means of shifting and/or scaling the variable  $x$ .

The authors define a *universal* set  $\mathbb{U}_d$  of at most  $1.1d \log^2(d)$  points on the complex plane such that Newton's iterations initiated at these points converge to *all roots of any polynomial*  $p(x)$  of (1).

The subsequent papers [BAS15], [BLS13], [S02], [S08], and [S13] decreased the cardinality of the set  $\mathbb{S}_d$  to  $O(d(\log(\log(d)))^2)$ , and it was proved in [BAS15] that one can approximate all roots of  $p(x)$  within relative errors of at most  $1/2^b$  by applying an expected overall number  $O(d^2 \log^4(d) + db)$  of Newton's iterations initialized at the points of that set.

In the paper [SSa] Newton's iterations initialized at just  $m_d = O(d)$  points of a *quasi-universal set*  $\mathbb{Q}_d$  and applied to any polynomial  $p(x)$  of (1) converged to *almost all* its roots, except for a small fraction of  $w = w(p)$  roots ( $w < 0.001 d$  for  $d < 2^{17}$  and  $w < 0.01 d$  for  $d < 2^{20}$ ). We call these roots *wild* and w.l.o.g. denote them  $x_1, \dots, x_w$  (otherwise we would re-enumerate the roots); we call the other roots  $x_{w+1}, \dots, x_d$  *tame*.

We propose three directions to the approximation of the wild roots without increasing the overall asymptotic computational cost. Our recipes for enhancing the power of Newton's and/or other functional iterations for polynomial root-finding by means of combining them successively or concurrently under various maps of the variable can be of independent interest.

## 2 Taming the Wild Roots by Means of Deflation

Our first recipe is *deflation*: we apply Newton's iterations to the polynomial

$$q(x) = \sum_{i=0}^w q_i x^i = p_d \prod_{j=1}^w (x - x_j), \quad p_d \neq 0. \quad (4)$$

In our first algorithm the deflation is explicit: we compute the coefficients of  $q(x)$  and then apply to it Newton's iteration. Unless the number of wild roots is small, this technique can be prone to numerical problems, but our second algorithm avoids computation of the coefficients of  $q(x)$ : it applies implicit deflation by exploiting the well-known identity

$$1/N_p(x) = \sum_{j=1}^n \frac{1}{x - x_j}. \quad (5)$$

**Algorithm 1.** *Explicit Deflation.*

INPUT: The tame roots  $x_w, \dots, x_d$  of a polynomial  $p(x)$  of (2); the quasi-universal set  $\mathbb{Q}_w = \{z_1, \dots, z_{m_w}\}$ , and a black-box program  $\text{EVAL}_p$  that evaluates a polynomial  $p(x)$  of (2) at a complex point  $x$ .

INITIALIZATION: Fix the integer  $h = \lceil \log_2 w \rceil$ , such that  $w < 2^h \leq 2w$ , write  $m = 2^h$  and  $\theta_m = \exp(2\pi\sqrt{-1}/m)$  (so that  $\theta_m$  is a primitive  $m$ th root of unity), and compute all  $m$ th roots of unity,  $1, \theta_m, \theta_m^2, \dots, \theta_m^{m-1}$ . Write

$$s(x) = \prod_{j=w+1}^d (x - x_j) = p(x)/q(x). \quad (6)$$

COMPUTATIONS: 1. Compute the values  $p(\theta_m^k)$  and  $s(\theta_m^k)$ ,  $k = 0, 1, \dots, m-1$ .  
 2. Compute the ratios  $p(\theta_m^k)/s(\theta_m^k)$ ,  $k = 0, 1, \dots, m-1$ , for  $q(x)$  of (4).  
 3. Interpolate to the polynomial  $q(x) = p(x)/s(x)$ .  
 4. Compute and output the values  $N_q(z_j) = q(z_j)/q'(z_j)$ , for  $j = 1, \dots, m_w$ .

**Complexity of Algorithm 1:** at Stage 1 we call the program  $\text{EVAL}_p$   $m$  times and in addition perform  $(2d - 2w - 1)m$  arithmetic operations; Stage 2 involves  $m$  divisions; at Stage 3 we perform  $(1.5 \log_2(m) + 1)m$  arithmetic operations (by using Inverse FFT), and Stage 4 involves  $(4w - 2)m_w$  arithmetic operations.

**Algorithm 2.** *Implicit Deflation.*

INPUT: The tame roots  $x_w, \dots, x_d$  of a polynomial  $p(x)$  of (2); the quasi-universal set  $\mathbb{Q}_w = \{z_1, \dots, z_{m_w}\}$ , and a black-box program  $\text{EVAL}_{p'/p}$  that evaluates the ratio  $p'(x)/p(x)$  at a complex point  $x$ .

COMPUTATIONS: 1. Compute the ratios  $r_k = p'(z_k)/p(z_k)$ , for  $k = 1, \dots, m_w$ .  
 2. Compute the values  $s_k = \sum_{j=m_w+1}^d \frac{1}{z_k - x_j}$ , for  $k = 1, \dots, m_w$ .  
 3. Compute and output the values  $N_q(z_k) = \frac{q(z_k)}{q'(z_k)} = \frac{1}{r_k - s_k}$ , for  $k = 1, \dots, m_w$ .<sup>1</sup>

At Stage 1 we call the program  $\text{EVAL}_{p'/p}$   $m_w$  times.

Stage 2 involves  $(d - m_w)m_w$  divisions and  $(2d - 2m_w - 1)m_w$  additions and subtractions.

At Stage 3 we perform  $m_w$  subtractions and  $m_w$  divisions.

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<sup>1</sup>D. A. Bini proposed to improve numerical stability of this iteration by scaling this expression as follows:

$$N_q(z_k) = \frac{1/r_k}{1 - s_k/r_k} = \frac{N_q(z_k)}{1 - s_k N_q(z_k)}.$$

### 3 Taming the Wild Roots by Means of Functional Iterations

Another natural approach is to combine Newton's method with other functional iterations for root-finding. A number of iterative processes, most notably the Weierstrass's [W03] (frequently attributed to its later rediscoveries, e.g., by Durand [D60] and Kerner [K66]) and Ehrlich–Aberth's [E67], [A73], globally converge very fast in practice, although this empirical observation has no adequate formal support.

One can extend the progress in [SSa] by substituting the tame roots into the Weierstrass's and Ehrlich–Aberth's iterations, which would greatly simplify their computations. Let us specify this *implicit deflation* for the latter iterations:

$$z_j^{(k+1)} = z_j^{(k)} - \frac{1}{u_j(z_j^{(k)})} \text{ for } u_j(x) = \frac{1}{N_p(x) - \sum_{h \neq j} \frac{1}{x_h - x}} \text{ and } j = 1, \dots, d. \quad (7)$$

Given the tame roots  $x_j$  of  $p(x)$ , for  $j = w+1, \dots, d$ , we only need to apply this iteration for the approximation of the remaining wild roots  $x_1, \dots, x_w$ , that is, we only need to apply (7) for  $j = 1, \dots, w$ , and we can adjust accordingly the initialization of these iterations in [B96], [BF00], and [BR14].

Similarly one can implicitly deflate other functional iterations for roots of  $p(x)$  such as the Gauss-Seidel's and Werner's accelerated variations of the Ehrlich–Aberth's and Weierstrass's iterations (cf. [BR14] and [W82]).

### 4 Taming the Wild Roots by Means of Mapping the Variable

Our next techniques can complement or replace the iterative algorithms of the previous sections in order to approximate all wild roots of a polynomial  $p(x)$  of (2). Namely we propose to apply Newton's iterations to the polynomials

$$v(z) = v_{a,b,c}(z) = (z+c)^d p\left(a + \frac{b}{z+c}\right)$$

for various triples of complex scalars  $a$ ,  $b \neq 0$ , and  $c$ , whose number, however, must be limited in order to control the overall computational cost.

#### Algorithm 3.

INITIALIZATIONS: Fix a triple  $a$ ,  $b \neq 0$ , and  $c$  defining a polynomial  $v(z) = v_{a,b,c}(z)$ .

COMPUTATIONS: 1. Shift and/or scale the variable  $z$  in order to move all roots of this polynomial into the unit disc  $D(0, 1) = \{z : |z| = 1\}$ .

2. Apply Newton's iteration to the resulting polynomial by using initialization at quasi-universal set of [SSa]. (In order to simplify the notation, assume that this is still the same polynomial  $v(z)$ .)

3. Avoid the computation of its coefficients by expressing the Newton's ratios by applying the following equations:

$$\frac{1}{N_v(z)} = \frac{v'(z)}{v(z)} = \frac{d}{z+c} - \frac{b}{(z+c)^2 N(z)} \text{ for } N(z) = N_{p(a+b/(z+c))}(z). \quad (8)$$

4. Having approximated a root  $z_j = \frac{b}{x_j - a} - c$  of  $v(z)$  for any  $j$ , readily recover the root of  $p(x)$ ,

$$x_j = a + \frac{b}{z_j + c}. \quad (9)$$

One can accelerate this algorithm by combining it with Algorithm 1 or 2.

In the particular case where  $a = c = 0$  and  $b = 1$ , the above expressions are simplified as follows:  $z = 1/x$ ;  $v(z)$  turns into the reverse polynomial of  $p(x)$ ,

$$v(z) = p_{\text{rev}}(z) = \sum_{i=0}^d p_{d-i} z^i = z^d p(1/z), \quad (10)$$

such that  $p_{\text{rev}}(x) = p_0 \prod_{j=1}^d (x - 1/x_j)$  if  $p_0 \neq 0$ , and

$$\frac{1}{N_v(z)} = \frac{v'(z)}{v(z)} = \frac{d}{z} - \frac{1}{z^2 N(z)} \text{ for } N(z) = N_{p(1/z)}(z).$$

We can hope to obtain all roots of  $p(x)$  by applying Newton's iterations for a reasonable number of triples of  $a$ ,  $b$  and  $c$ , but we can also extend our approach by using more general rational maps  $y = r(x)$  (cf., e.g., [MP00]).

For a simple example, consider the Dandelin's root-squaring map [H59]:

$$u(y) = (-1)^d p(\sqrt{y}) p(-\sqrt{y}) = \prod_{j=1}^d (y - x_j^2). \quad (11)$$

In this case one should either assume that a polynomial  $p(x)$  of (2) is monic or scale it to make it monic; then one can express the Newton's ratio as follows:

$$N_u(y) = \frac{1}{2} (-1)^d y^{-1/2} \left( \frac{1}{N_p(\sqrt{y})} - \frac{1}{N_p(\sqrt{-y})} \right).$$

Note that under map (11) the roots lying in the unit disc  $D(0, 1)$  stay in it.

Having approximated the  $n$  roots  $y_1, \dots, y_n$  of the polynomial  $u(y)$ , we can readily recover the  $n$  roots  $x_1, \dots, x_n$  of the polynomial  $p(x)$  from the  $2n$  values  $\pm\sqrt{y_j}$ ,  $j = 1, \dots, n$ .

We can combine the above maps recursively (a limited number of times, in order to control the overall computational cost) and then recover the roots from their images in these rational maps by extending the lifting/descending techniques of [P95], [P02].

The approach can be applied independently of the algorithms of the previous sections or can be combined with them, particularly with implicit deflation, in

order to decrease the computational cost or to extend their power to a larger domain of inputs.

For practical benefits, the selected functional iterations for the selected polynomials  $p(x)$ ,  $u(y)$ , and  $v(z)$  can be implemented concurrently, with minimal need for processor communication and synchronization, as long as sufficiently many processors are available.

## 5 Conclusions

Some of our techniques may be of independent interest. Combination of various functional root-finding iterations towards their faster convergence in wider input domains is a well-known challenge. In order to meet this challenge, one can first transform an input polynomial  $p(x)$  by means of the maps  $x = a + \frac{b}{z+c}$  for various triples of  $a$ ,  $b$ , and  $c$  or by means of more general rational maps  $x = x(y)$ , then successively or concurrently apply the selected functional iterations to the resulting polynomials, and finally recover the roots of  $p(x)$  from the tame roots output by these iterations.

For a specific application of such maps, consider another important challenge, of the approximation of the roots isolated in the unit disc  $D(0, 1)$  on the complex plane.

Both Weierstrass's and Ehrlich–Aberth's iterations do not seem to do well for this task when the number,  $\nu$ , of the roots in the disc is much smaller than  $d$ . Indeed in this case Newton's and other functional iterations (cf. [MP07] and [MP13, Chapter 9]) promise to accelerate the solution by a factor of  $d/\nu$ . For a formal support of their global convergence, however, we cannot bluntly apply the techniques of the papers [HSS01], [BAS15], [BLS13], [S02], [S08], [S13], and [SSa], because they exploit the large size of the areas about the orbits connecting the roots to the infinity. The following algorithm may alleviate this difficulty.

### Algorithm 4.

- COMPUTATIONS:
1. Apply a limited number of Dandelin's root squaring steps. [Then all superfluous roots of  $p(x)$ , lying in the exterior of that disc (denote them  $x_{\nu+1}, \dots, x_d$ ) are moved farther from the disc  $D(0, 1)$ , while the other roots,  $x_1, \dots, x_\nu$ , stay in this disc.]
  2. Apply the map  $y = 1/z$ . [It moves all the superfluous roots of  $p(x)$  into a small disc inside  $D(0, 1)$ , while moving the roots  $x_1, \dots, x_\nu$  into the exterior of the disc  $D(0, 1)$ .]
  3. Move all roots into the unit disc  $D(0, 1)$  by applying shift and/or scaling of the variable. [This keeps the images of the roots  $x_1, \dots, x_\nu$  strongly isolated in a small disc inside the disc  $D(0, 1)$ .]
  4. Apply Newton's iteration to the resulting polynomial by using initialization at the universal or quasi-universal set.
  5. Recover the roots of  $p(x)$  from their images computed by these iterations.

We can conjecture that the iterations would first converge to the images of the roots  $x_1, \dots, x_\nu$  of the polynomial  $p(x)$ , thus achieving a desired acceleration by a factor of  $d/\nu$  or perhaps  $d/\nu^2$ . This conjecture can be tested empirically, but one can also try to yield its formal support by extending the study in [HSS01], [BAS15], [BLS13], [S02], [S08], [S13], and [SSa].

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